2,3,4-Trimethylpentane

565-75-3 | DTXSID6060343

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 252

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 7.35e-01

Nearest Neighbors from the Training Set

Image not found
Camphene
Measured: 955
Predicted: 598

Image not found
4-Vinylcyclohexene
Measured: 166
Predicted: 158

Image not found
Dibenzothiophene
Measured: 1120
Predicted: 84.5

Image not found
5-Ethylidene-2-norbornene
Measured: 110
Predicted: 134

Image not found
Styrene
Measured: 13.5
Predicted: 32.7